

tetrahedra,  $[\text{AlCl}(\text{CH}_3\text{CN})_5]^{2+}$  octahedra and isolated  $\text{CH}_3\text{CN}$  molecules.

Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and complete geometry have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55614 (61 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: DU1009]

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## Structures of Perfragilin A and B

SAFIA KHALIL RIZVI, M. B. HOSSAIN AND  
D. VAN DER HELM

Department of Chemistry and Biochemistry,  
Oklahoma University, Norman, Oklahoma 73019, USA

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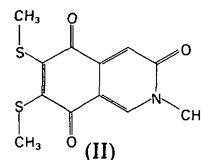
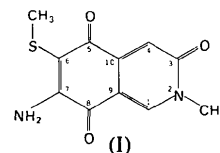
### Abstract

The two perfragilins both have a similar backbone (an isoquinolinetrione skeleton) but differ in their

substitution pattern at C(6) and C(7); perfragilin A has a thiomethyl group at C(6) and amide group at C(7), whereas perfragilin B has a thiomethyl group at both these positions. The effects of these substituents are reflected in the bond distances and bond angles, particularly in the benzoquinone segments of the molecules. The amide group in perfragilin A leads to a resonance structure and a planar isoquinoline ring system [r.m.s. deviation 0.026 (2) Å]. The presence of the two thiomethyl groups in perfragilin B causes the isoquinoline ring system to exhibit significant deviations from planarity [r.m.s. deviation 0.067 (1) Å].

### Comment

Perfragilin A and B [(I) and (II) respectively; see scheme below] are two new metabolites from a bryozoan, *Membranipora perfragilis* (Schmitz, DeGuzman, Choi, Hossain, Rizvi & van der Helm, 1990). Both compounds show cytotoxic activity on P388 murine leukemia cells with compound (II) nearly 20 times more active than (I) (Choi, Schmitz & van Altena, 1992). The perfragilins are derivatives of basic isoquinolinetrione and bear a close resemblance to mimosamycin which is produced by *Streptomyces lavendulae* (Fukumi, Kurihara, Hata, Tamura, Mishima, Kubo & Arai, 1977; Hata, Fukumi, Sato, Aiba & Tamura, 1978). The novel feature of the perfragilins is the presence of a thiomethyl group in place of the methoxy and methyl groups found in mimosamycin. It has recently been observed in some naturally occurring alkaloids (varamines and diplamine) that the cytotoxicity of compounds with a similar ring structure is increased by an order of magnitude by the introduction of a thiomethyl group (Charyulu, McKee & Ireland, 1989). An additional thiomethyl group in perfragilin B enhances its cytotoxicity, indicating that the thiomethyl group may play an important role in bioactivity. The structure determination of the two compounds was undertaken to establish the chemical structures of the two perfragilins and to obtain a better understanding of the effect of structural change on biological activity.



The final atomic parameters of the non-H atoms of the two compounds are given in Table 1, and bond distances and angles in Table 2. Perspective *ORTEP* (Johnson, 1965) drawings of perfragilin A and B are shown in Fig. 1. The effects of the amide and thio substituent groups in place of the methoxy and methyl groups in mimosamycin are evident in some of the bond distances and bond angles, particularly in the *p*-benzoquinone segment of the molecular backbone. In perfragilin A, the C(5)—C(6) bond [1.438 (2) Å] is 0.059 (2) Å shorter than the corresponding bond in perfragilin B while both the C(6)—C(7) and C(7)—C(8) bonds are significantly longer [0.023 (3) and 0.028 (3) Å respectively]. The C(5)—C(6) bond in perfragilin A is 0.023 (6) Å shorter and the C(6)—C(7) and C(7)—C(8) bonds 0.039 (6) and 0.013 (6) Å longer than those in mimosamycin (Hata *et al.*, 1978). The C(7)—N(16) bond [1.331 (2) Å] is also considerably shorter than a normal C(*sp*<sup>2</sup>)—N single bond (1.39 Å). These features indicate that perfragilin A has a resonance structure consisting of (I) and a form in which the double bond is shifted from C(6)—C(7) to C(5)—C(6). A similar resonance structure has also been observed in several amino-benzoquinone derivatives (Rettig & Trotter, 1975; Kulpe, 1969). In perfragilin B where the amide group is replaced by a thiomethyl group, the C(5)—C(6) and C(6)—C(7) bonds [1.497 (1) and 1.367 (2) Å] are only slightly different from those in mimosamycin [1.500 (8) and 1.351 (8) Å].

The ten-membered isoquinoline skeleton in perfragilin A is essentially planar with individual atoms

showing r.m.s. deviations of 0.026 (2) Å from the least-squares plane. Both the amide N atom and the S atom [deviations of 0.013 (2) and 0.033 (1) Å respectively] lie on the plane. In perfragilin B, the isoquinoline ring shows noticeable deviations from planarity [r.m.s. deviation 0.067 (1) Å]. The overall backbone is bent in the middle with a dihedral angle of 5.5 (3)° between the benzoquinone and pyridone rings. The two S atoms in perfragilin B lie out of the plane [deviations of 0.185 (1) and 0.152 (1) Å for S(14) and S(16) respectively]. All the carbonyl groups also deviate significantly from the ring plane [O(12) by 0.164 (1), O(13) by 0.295 (1) and O(17) by 0.254 (1) Å]. In both compounds, the pyridone ring is planar and the bond distances indicate some delocalization.

The thiomethyl groups show varied conformations. The methyl carbon C(15) in (I) lies out of the backbone plane (inclination angle of about 60°). The methyl C(18) in perfragilin B has a similar orientation as that in compound (I) (inclination of 55°), but the methyl carbon C(15) lies very close to the backbone plane (inclination of 18°). This orientation of the C(6) thiomethyl group in (II) leads to considerable steric strain as indicated by the enlargement of the angles C(5)—C(6)—S(14) and C(6)—S(14)—C(15) from 118.0 (1) and 101.9 (1)° respectively (I) to 122.0 (1) and 108.9 (1)° (II). The S—C(methyl) distance in the nearly coplanar thiomethyl group [1.789 (2) Å] is distinctly shorter than the corresponding bonds in the thiomethyl groups which are out of the plane [1.812 (2) in (I) and 1.806 (2) Å in II]. Bond-length shortening of a similar nature has been observed for the coplanar methoxy group in dimethoxyquinone (Silverman, Stam-Thole & Stam, 1971). In both structures, the molecules are packed in layers. In perfragilin A, each molecule is linked to two of its centrosymmetrically related neighbors through a strong N—H...S hydrogen bond [N(16)...S(14)(1 - x, 1 - y, 2 - z) = 3.317 (2) Å] and a weaker N—H...O hydrogen bond [N(16)...O(17)(2 - x, 1 - y, 2 - z) = 3.013 (2) Å].

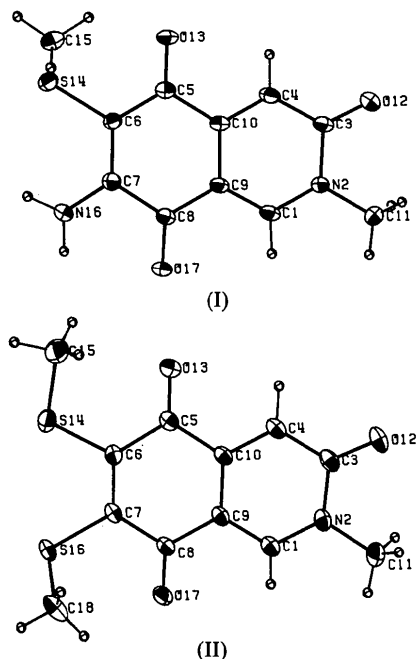


Fig. 1. Perspective *ORTEP* plots of (I) and (II) with atom numbering. Thermal ellipsoids are shown at 50% probability.

## Experimental

### Compound (I)

#### Crystal data

C<sub>11</sub>H<sub>10</sub>N<sub>2</sub>O<sub>3</sub>S

*M<sub>r</sub>* = 250.3

Triclinic

*P*1

*a* = 8.812 (2) Å

*b* = 8.500 (3) Å

*c* = 8.377 (3) Å

$\alpha$  = 85.61 (3)°

$\beta$  = 111.15 (3)°

$\gamma$  = 114.28 (3)°

Mo *K* $\alpha$  radiation

$\lambda$  = 0.71073 Å

Cell parameters from 48

reflections,

$\lambda$  = 0.70930 Å

$\theta$  = 11–19°

$\mu$  = 0.30 mm<sup>-1</sup>

*T* = 163 K

Needle

0.35 × 0.05 × 0.05 mm

$V = 531.5 \text{ \AA}^3$   
 $Z = 2$   
 $D_x = 1.563 \text{ Mg m}^{-3}$

**Data collection**

CAD-4 diffractometer  
 $\omega$ - $2\theta$  scans  
 2188 measured reflections  
 2188 independent reflections  
 1751 observed reflections  
 $[I \geq 2\sigma(I)]$   
 $\theta_{\max} = 26.5^\circ$

**Refinement**

Refinement on  $F$   
 Final  $R = 0.041$   
 $wR = 0.040$   
 $S = 1.92$   
 1751 reflections  
 194 parameters  
 All H-atom parameters re-  
 fined

**Compound (II)****Crystal data**

$\text{C}_{12}\text{H}_{11}\text{NO}_3\text{S}_2$   
 $M_r = 281.3$   
 Triclinic  
 $P\bar{1}$   
 $a = 6.915 (2) \text{ \AA}$   
 $b = 9.860 (3) \text{ \AA}$   
 $c = 9.924 (3) \text{ \AA}$   
 $\alpha = 111.22 (2)^\circ$   
 $\beta = 99.70 (2)^\circ$   
 $\gamma = 102.24 (2)^\circ$   
 $V = 593.7 \text{ \AA}^3$   
 $Z = 2$   
 $D_x = 1.573 \text{ Mg m}^{-3}$

**Data collection**

CAD-4 diffractometer  
 $\omega$ - $2\theta$  scans  
 2408 measured reflections  
 2408 independent reflections  
 2267 observed reflections  
 $[I \geq 2\sigma(I)]$   
 $\theta_{\max} = 75^\circ$

**Refinement**

Refinement on  $F$   
 Final  $R = 0.039$   
 $wR = 0.055$   
 $S = 2.41$   
 2267 reflections  
 207 parameters  
 All H-atom parameters re-  
 fined

Pink

$h = 0 \rightarrow 11$   
 $k = -10 \rightarrow 10$   
 $l = -10 \rightarrow 10$   
 3 standard reflections  
 frequency: 120 min  
 intensity variation: 2.9%

$w = 1/\sigma^2(I)$   
 $(\Delta/\sigma)_{\max} = 0.01$   
 $\Delta\rho_{\max} = 0.26 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = 0.43 \text{ e \AA}^{-3}$   
 Atomic scattering fac-  
 tors from *SHELX76*  
 (Sheldrick, 1976)

Cu  $K\alpha$  radiation  
 $\lambda = 1.54178 \text{ \AA}$   
 Cell parameters from 48  
 reflections,  
 $\lambda = 1.54051 \text{ \AA}$   
 $\theta = 22\text{--}42^\circ$   
 $\mu = 3.94 \text{ mm}^{-1}$   
 $T = 163 \text{ K}$   
 Thick plate  
 $0.22 \times 0.16 \times 0.10 \text{ mm}$   
 Pink

$h = 0 \rightarrow 8$   
 $k = -12 \rightarrow 12$   
 $l = -12 \rightarrow 12$   
 3 standard reflections  
 frequency: 120 min  
 intensity variation: 3.6%

$w = 1/\sigma^2(F_o)$   
 $(\Delta/\sigma)_{\max} = 0.06$   
 $\Delta\rho_{\max} = 0.49 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = 0.42 \text{ e \AA}^{-3}$   
 Atomic scattering factors  
 from *SHELX76*

Table 1. Fractional atomic coordinates and equivalent isotropic thermal parameters ( $\text{\AA}^2$ )

	$U_{\text{eq}} = \frac{1}{3} \sum_i \sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i \cdot \mathbf{a}_j$			$U_{\text{eq}}$
	x	y	z	
(I)				
S(14)	0.42819 (9)	0.62148 (8)	0.77660 (8)	0.0221 (3)
O(12)	0.8561 (2)	0.9534 (2)	0.1098 (2)	0.0301 (8)
O(13)	0.4515 (2)	0.7635 (2)	0.4459 (2)	0.0274 (8)
O(17)	0.9989 (2)	0.5869 (2)	0.7941 (2)	0.0256 (7)
N(2)	0.9852 (2)	0.8171 (2)	0.3280 (2)	0.0185 (8)
N(16)	0.7520 (3)	0.5331 (3)	0.9278 (3)	0.0249 (9)
C(1)	0.9916 (3)	0.7411 (3)	0.4766 (3)	0.0188 (9)
C(3)	0.8489 (3)	0.8742 (3)	0.2375 (3)	0.020 (1)
C(4)	0.7126 (3)	0.8327 (3)	0.3089 (3)	0.021 (1)
C(5)	0.5783 (3)	0.7269 (3)	0.5296 (3)	0.019 (1)
C(6)	0.5963 (3)	0.6569 (3)	0.6938 (3)	0.0180 (9)
C(7)	0.7344 (3)	0.6066 (3)	0.7798 (3)	0.0191 (9)
C(8)	0.8791 (3)	0.6324 (3)	0.7109 (3)	0.0184 (9)
C(9)	0.8681 (3)	0.7121 (3)	0.5494 (3)	0.0170 (9)
C(10)	0.7216 (3)	0.7594 (3)	0.4596 (3)	0.0177 (9)
C(11)	1.1241 (4)	0.8518 (4)	0.2559 (4)	0.025 (1)
C(15)	0.4535 (4)	0.8402 (3)	0.8109 (4)	0.024 (1)
(II)				
S(14)	-0.00899 (7)	0.71594 (6)	0.65302 (6)	0.0351 (2)
S(16)	0.38491 (6)	0.91518 (5)	0.64515 (5)	0.0266 (2)
O(12)	0.6592 (2)	0.5972 (1)	1.2763 (1)	0.0282 (5)
O(13)	0.0603 (2)	0.6303 (1)	0.9255 (1)	0.0284 (5)
O(17)	0.7441 (2)	0.9754 (1)	0.8916 (1)	0.0272 (5)
N(2)	0.8051 (2)	0.7563 (1)	1.1773 (1)	0.0220 (5)
C(1)	0.7895 (3)	0.8252 (2)	1.0817 (2)	0.0214 (6)
C(3)	0.6332 (3)	0.6604 (2)	1.1907 (2)	0.0225 (6)
C(4)	0.4376 (3)	0.6440 (2)	1.0984 (2)	0.0218 (6)
C(5)	0.2175 (2)	0.6903 (2)	0.9042 (2)	0.0207 (6)
C(6)	0.2170 (2)	0.7463 (2)	0.7826 (2)	0.0210 (6)
C(7)	0.3938 (2)	0.8353 (2)	0.7773 (2)	0.0207 (6)
C(8)	0.5946 (2)	0.8799 (2)	0.8880 (2)	0.0198 (6)
C(9)	0.6045 (2)	0.8052 (2)	0.9913 (2)	0.0192 (5)
C(10)	0.4237 (2)	0.7124 (2)	1.0007 (2)	0.0189 (6)
C(11)	1.0075 (3)	0.7764 (2)	1.2694 (2)	0.0317 (7)
C(15)	-0.1971 (3)	0.5511 (3)	0.6365 (3)	0.0397 (8)
C(18)	0.5628 (4)	0.8416 (2)	0.5468 (2)	0.0332 (8)

Table 2. Bond lengths ( $\text{\AA}$ ) and angles ( $^\circ$ )

	(I)	(II)
S(16)—C(7)	-	1.757 (1)
S(16)—C(18)	-	1.806 (2)
S(14)—C(6)	1.763 (2)	1.741 (2)
S(14)—C(15)	1.812 (2)	1.789 (2)
C(1)—N(2)	1.351 (2)	1.355 (1)
C(1)—C(9)	1.361 (3)	1.363 (2)
N(2)—C(3)	1.422 (3)	1.412 (2)
C(3)—C(4)	1.436 (3)	1.441 (2)
C(3)—O(12)	1.227 (2)	1.234 (1)
C(4)—C(10)	1.355 (2)	1.369 (1)
C(5)—C(6)	1.438 (2)	1.497 (1)
C(5)—C(10)	1.496 (3)	1.501 (2)
C(5)—O(13)	1.235 (3)	1.213 (2)
C(6)—C(7)	1.390 (3)	1.367 (2)
C(7)—C(8)	1.513 (3)	1.485 (2)
C(7)—N(16)	1.331 (2)	-
C(8)—C(9)	1.456 (2)	1.464 (1)
C(8)—O(17)	1.230 (2)	1.228 (2)
C(9)—C(10)	1.440 (3)	1.423 (2)
N(2)—C(11)	1.469 (3)	1.467 (2)
C(4)—C(10)—C(9)	119.6 (2)	120.0 (1)
C(5)—C(6)—C(7)	121.4 (2)	120.7 (1)
C(5)—C(10)—C(9)	120.8 (1)	120.05 (8)
C(6)—S(14)—C(15)	101.94 (9)	108.90 (7)
C(6)—C(5)—C(10)	118.2 (2)	116.8 (1)
C(6)—C(5)—O(13)	122.7 (2)	122.4 (1)
C(6)—C(7)—C(8)	121.8 (2)	122.82 (9)
C(6)—C(7)—N(16)	123.8 (2)	-
C(6)—C(7)—S(16)	-	119.8 (1)

C(7)—C(8)—C(9)	117.3 (2)	116.9 (1)
C(7)—C(8)—O(17)	118.7 (2)	120.90 (9)
C(8)—C(7)—N(16)	114.4 (2)	-
C(8)—C(7)—S(16)	-	117.2 (1)
C(8)—C(9)—C(10)	120.2 (2)	121.3 (1)
C(9)—C(8)—O(17)	124.0 (2)	122.2 (1)
N(2)—C(1)—C(9)	122.8 (2)	121.5 (1)
C(10)—C(5)—O(13)	119.0 (1)	120.85 (9)
C(7)—S(16)—C(18)	-	101.13 (6)
S(14)—C(6)—C(5)	118.0 (1)	122.0 (1)
S(14)—C(6)—C(7)	120.5 (1)	117.10 (8)
C(1)—N(2)—C(3)	122.0 (2)	122.8 (1)
C(1)—N(2)—C(11)	121.4 (2)	120.1 (1)
C(1)—C(9)—C(8)	121.8 (2)	119.8 (1)
C(1)—C(9)—C(10)	117.9 (1)	118.89 (9)
N(2)—C(3)—C(4)	114.8 (1)	115.25 (8)
N(2)—C(3)—O(12)	119.4 (2)	119.4 (1)
C(3)—N(2)—C(11)	116.6 (1)	117.12 (9)
C(3)—C(4)—C(10)	122.7 (2)	121.5 (1)
C(4)—C(3)—O(12)	125.8 (2)	125.4 (1)
C(4)—C(10)—C(5)	119.6 (2)	120.0 (1)

Both compounds were crystallized from  $\text{CDCl}_3/\text{CF}_3\text{COOD}$ . The data sets were corrected for Lorentz and polarization effects but not for absorption. The structures were determined by direct methods using *MULTAN80* (Main, Fiske, Hull, Lessinger, Germain, Declercq & Woolfson, 1980) and refined by full-matrix least squares with *SHELX76*. In each case, the H atoms were located from the difference Fourier map and refined isotropically.

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Lists of structure factors, anisotropic thermal parameters, H-atom coordinates and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55458 (32 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: ST1006]

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## *N*-(4,6-Diméthylpyrid-2-yl)-2-(3-nitrophényl)acétamide

N. RODIER

*Laboratoire de Chimie minérale, Faculté des Sciences pharmaceutiques et biologiques, 5 Rue J.-B. Clément, 92296 Châtenay-Malabry CEDEX, France*

J.-M. ROBERT, S. ROBERT-PIESSARD ET G. LE BAUT

*Laboratoire de Chimie thérapeutique, Faculté de Pharmacie, 1 Rue Gaston-Veil, 44035 Nantes CEDEX, France*

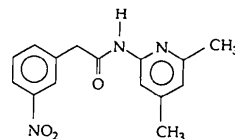
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## Abstract

The molecule of the title compound can be regarded as being composed of two parts, an *N*-(4,6-diméthylpyrid-2-yl)acetamide group and a 3-methylnitrobenzene group, which share the C(9) atom. The two parts are approximately planar. The least-squares planes through the pyridyl and phenyl rings make an angle of  $64.5(1)^\circ$ . An intramolecular hydrogen bond [C(3)—H(3)⋯O(18): 2.870(4) Å,  $114(3)^\circ$ ] forms a pseudo ring and contributes to the planarity of the *N*-(4,6-diméthylpyrid-2-yl)acetamide group. The molecules are linked together by the N(7)—H(7)⋯O(18<sup>i</sup>) hydrogen bond [ $i$   $x, \frac{1}{2} - y, \frac{1}{2} + z$ ; 2.859(3) Å,  $170(3)^\circ$ ]. They form two chains parallel to the *c* axis and related by a centre of symmetry.

## Commentaire

Le *N*-(4,6-diméthylpyrid-2-yl)-2-(3-nitrophényl)acétamide appartient à une famille de composés anti-inflammatoires dérivés de la 6-amino-2,4-lutidine. L'étude cristallographique a été entreprise dans le but de préciser la géométrie de sa molécule et de la comparer à celles des molécules actives de la même famille.



Les cycles *A* et *B* (Fig. 1) sont plans. Les valeurs du paramètre  $\chi^2$  relatives à leurs plans moyens respectifs *P*(*A*) et *P*(*B*) sont égales à 2 et à 12. N(7), C(8), C(9), C(16) et C(17) sont proches de *P*(*A*) dont O(18) est éloigné de 0,497(2) Å. L'angle de torsion